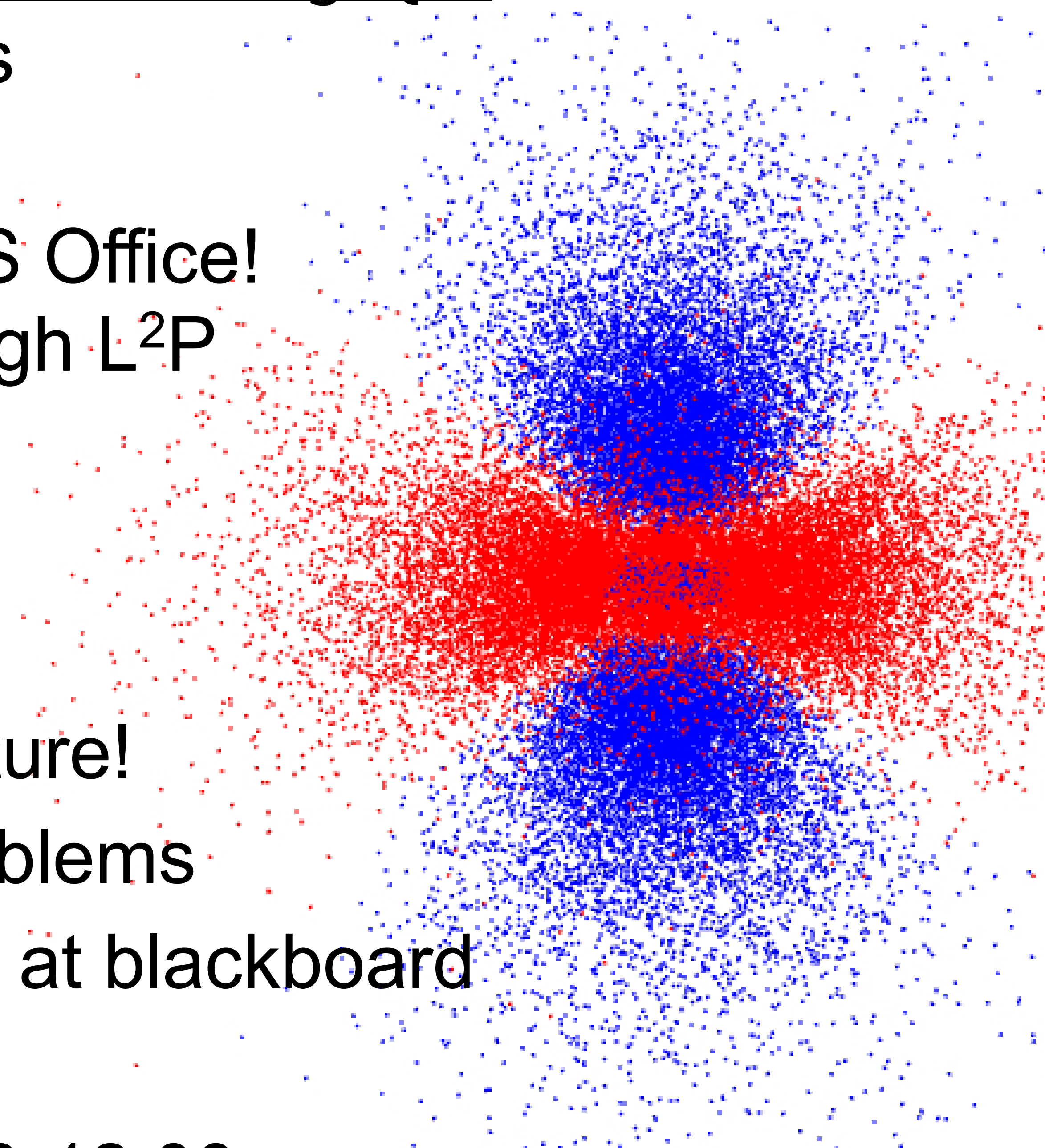
Applied Quantum Mechanics

lecture site: http://www.cond-mat.de/teaching/QM/
slides, links, exercises

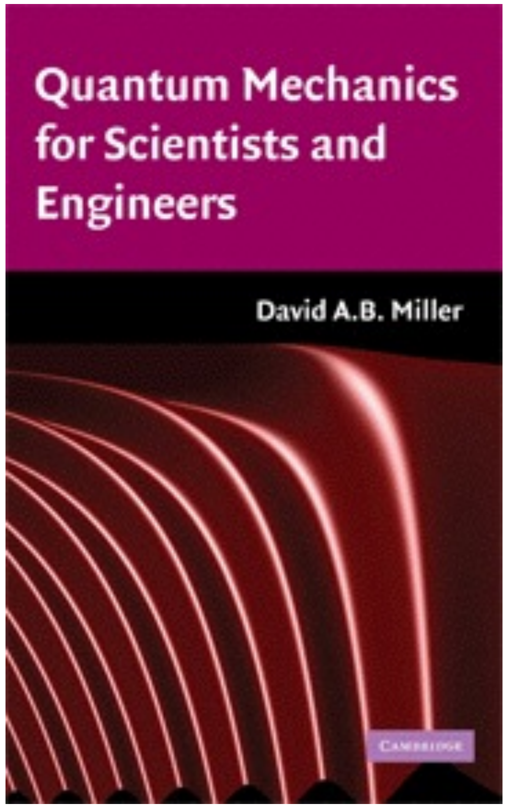
register for course through CAMPUS Office!
exercises and some material through L^{2}P

course policies:

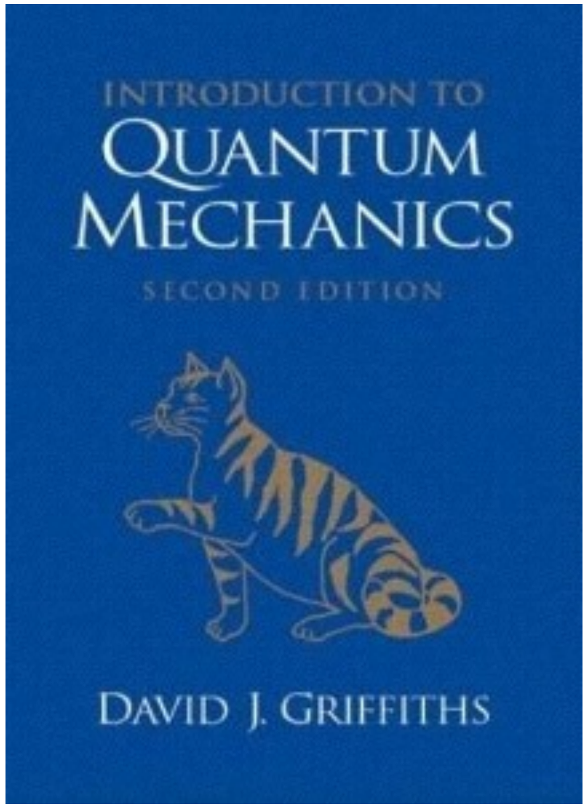
- exercises:
  - hand in (Hunter Sims) before lecture!
  - need to solve at least 50% of problems
  - prepare to present your solutions at blackboard
- exam:
  - final exam Thu 19 Feb 2015, 9:30-12:00



textbooks



D.A.B. Miller:
Quantum Mechanics for Scientists and Engineers
Cambridge Univ. Press



D.J. Griffiths:
Introduction to Quantum Mechanics
Pearson

F. Schwabl:
Quantum Mechanics

Springer

Matter is made of atoms

If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the *atomic hypothesis* (or the atomic *fact*, or whatever you which to call it) that *all things are made of atoms – little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.* In that one sentence, you will see, there is and *enormous* amount of information about the world, if just a little imagination and thinking are applied.

Lecture 1 of The Feynman Lectures on Physics, Vol. I (1961)

exercise

given
N_e electrons, N_i atomic nuclei of mass M_α und charge Z_α,
solve:

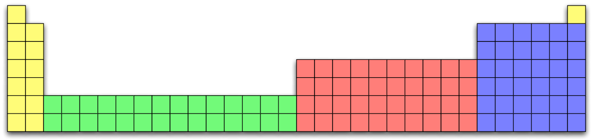
$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r}_1,\ldots,\vec{r}_{N_e};\vec{R}_1,\ldots,\vec{R}_{N_i};t) = H\,\Psi(\vec{r}_1,\ldots,\vec{r}_{N_e};\vec{R}_1,\ldots,\vec{R}_{N_i};t)$$

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N_e}\nabla_j^2 - \sum_{\alpha=1}^{N_i}\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \frac{1}{4\pi\epsilon_0}\sum_{j=1}^{N_e}\sum_{\alpha=1}^{N_i}\frac{Z_\alpha e^2}{|r_j - R_\alpha|} + \frac{1}{4\pi\epsilon_0}\sum_{j<k}^{N_e}\frac{e^2}{|r_j - r_k|} + \frac{1}{4\pi\epsilon_0}\sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|}$$

The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that exact applications of these laws lead to equations which are too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

P.M.A Dirac, *Proceedings of the Royal Society* **A123**, 714 (1929)

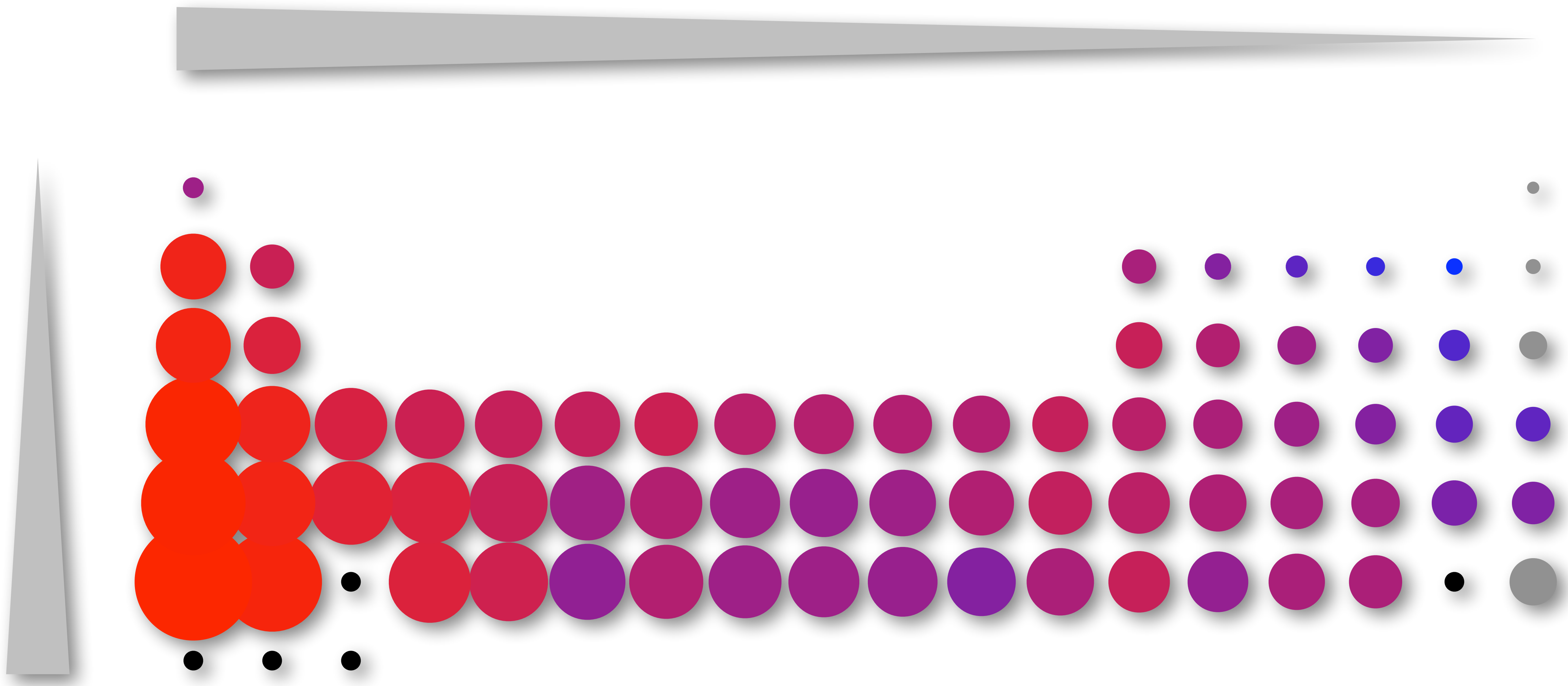
periodic table



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt									

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

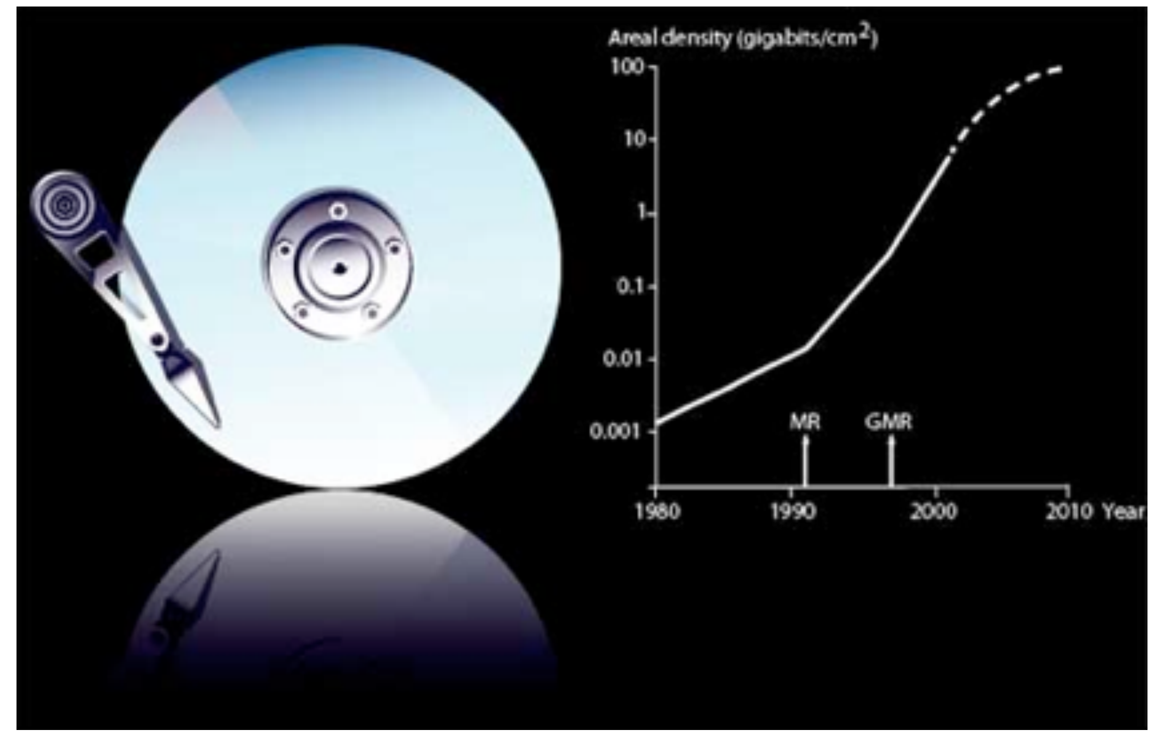
atomic radii

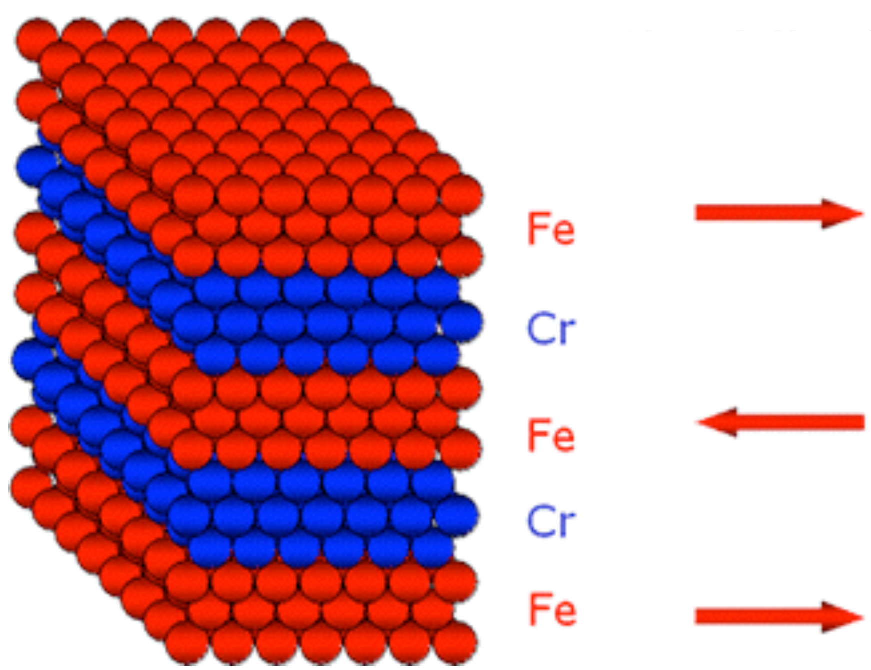


typical size 10^{-10} m = 1 Å

giant magnetoresistance

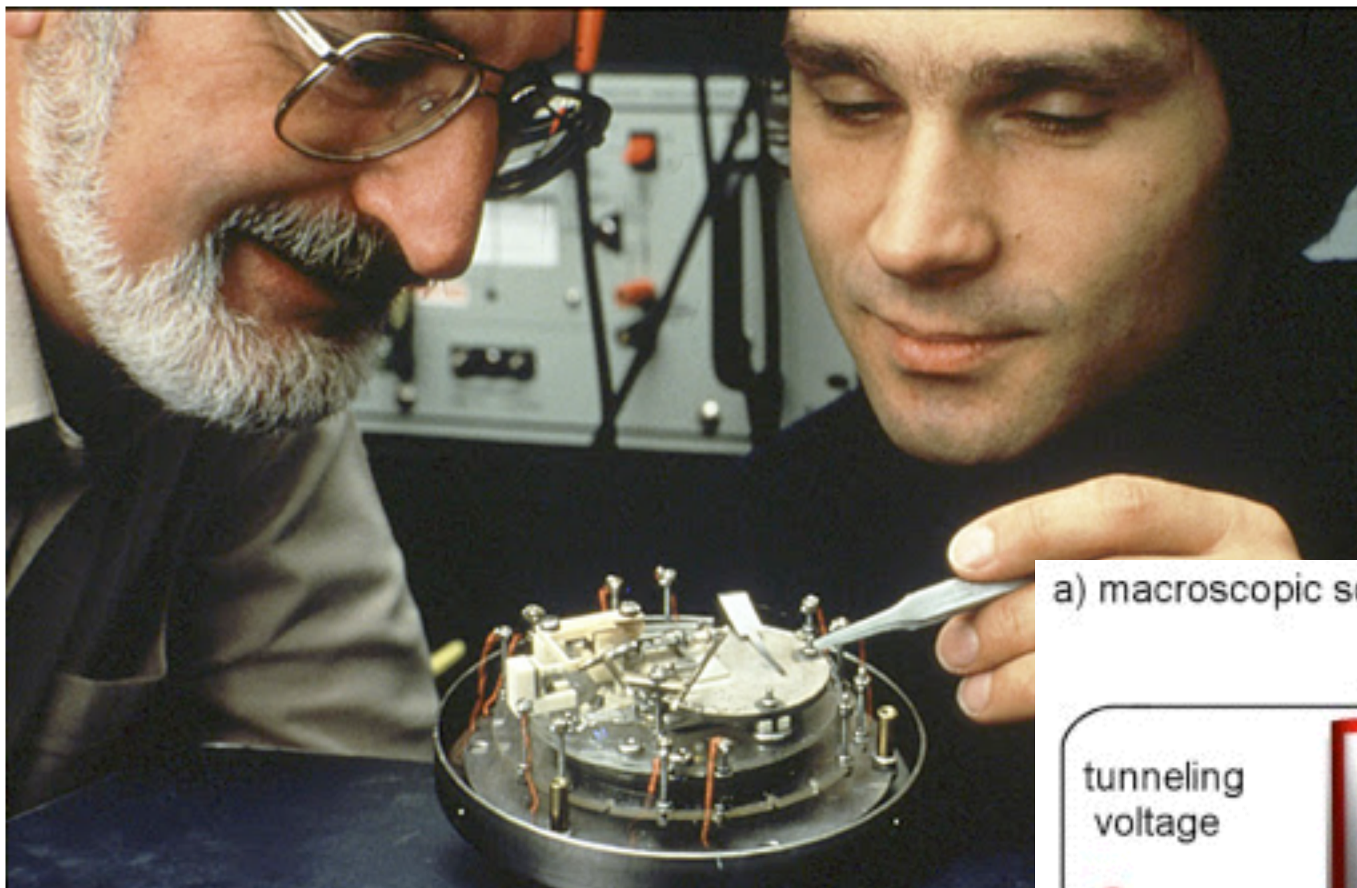
Peter Grünberg (Jülich) and Albert Fert (Paris), 1988
Nobel prize in Physics 2007

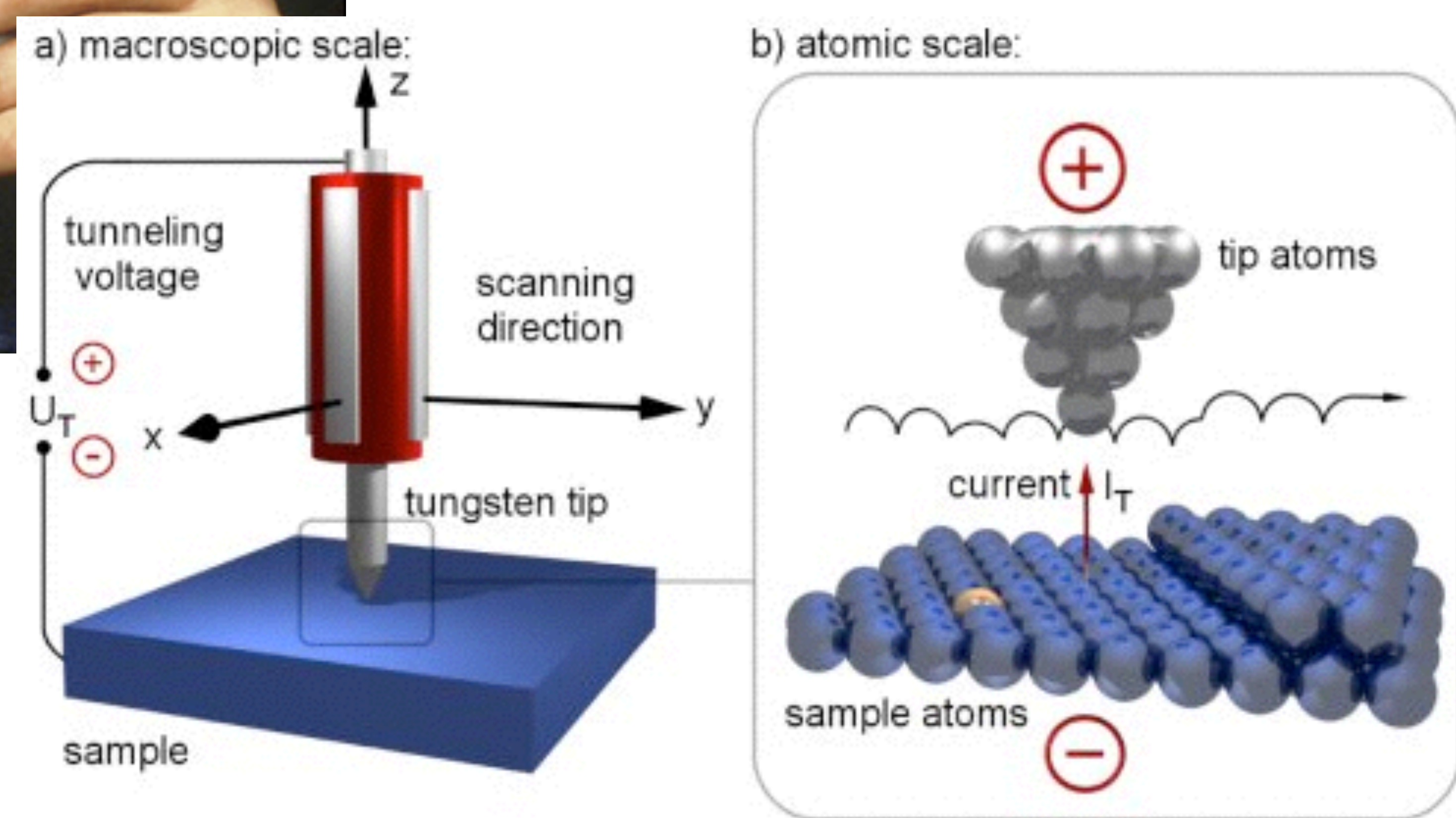




scanning tunneling microscope

Gerd Binnig and Heinrich Rohrer, IBM Rüschlikon, 1981
Nobel Prize in Physics 1986



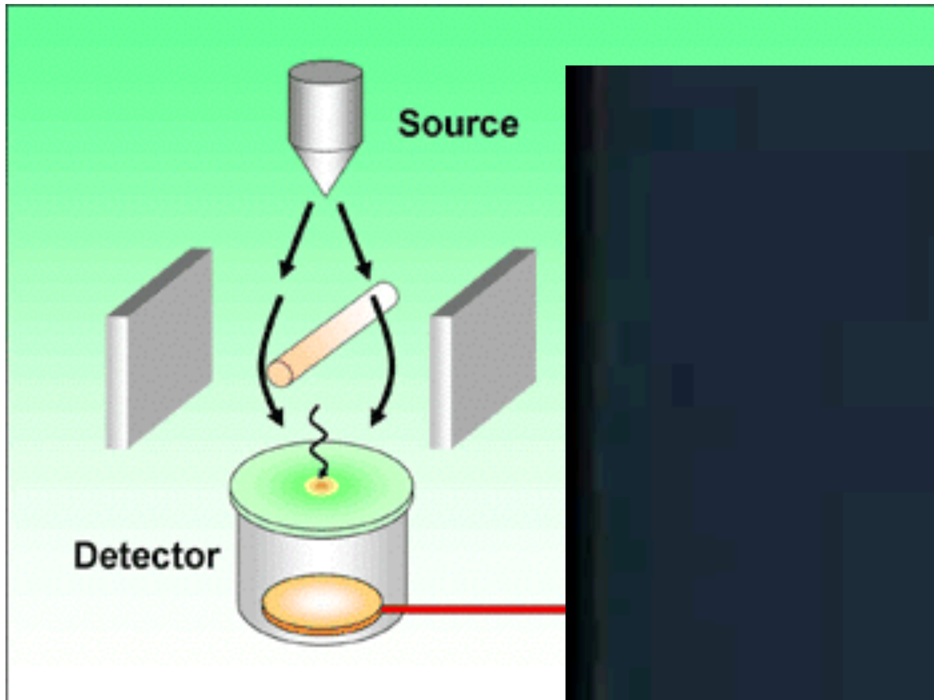


scanning tunneling microscope

seeing and manipulating atoms

http://www2.fz-juelich.de/ibn/microscope_e

double-slit experiment with electrons



http://www.hitachi.com/rd/research/em/doubleslit.html

see also: R.P. Feynman: Feynman Lectures on Physics, Vol. 3
Ch. 1: Quantum Behavior

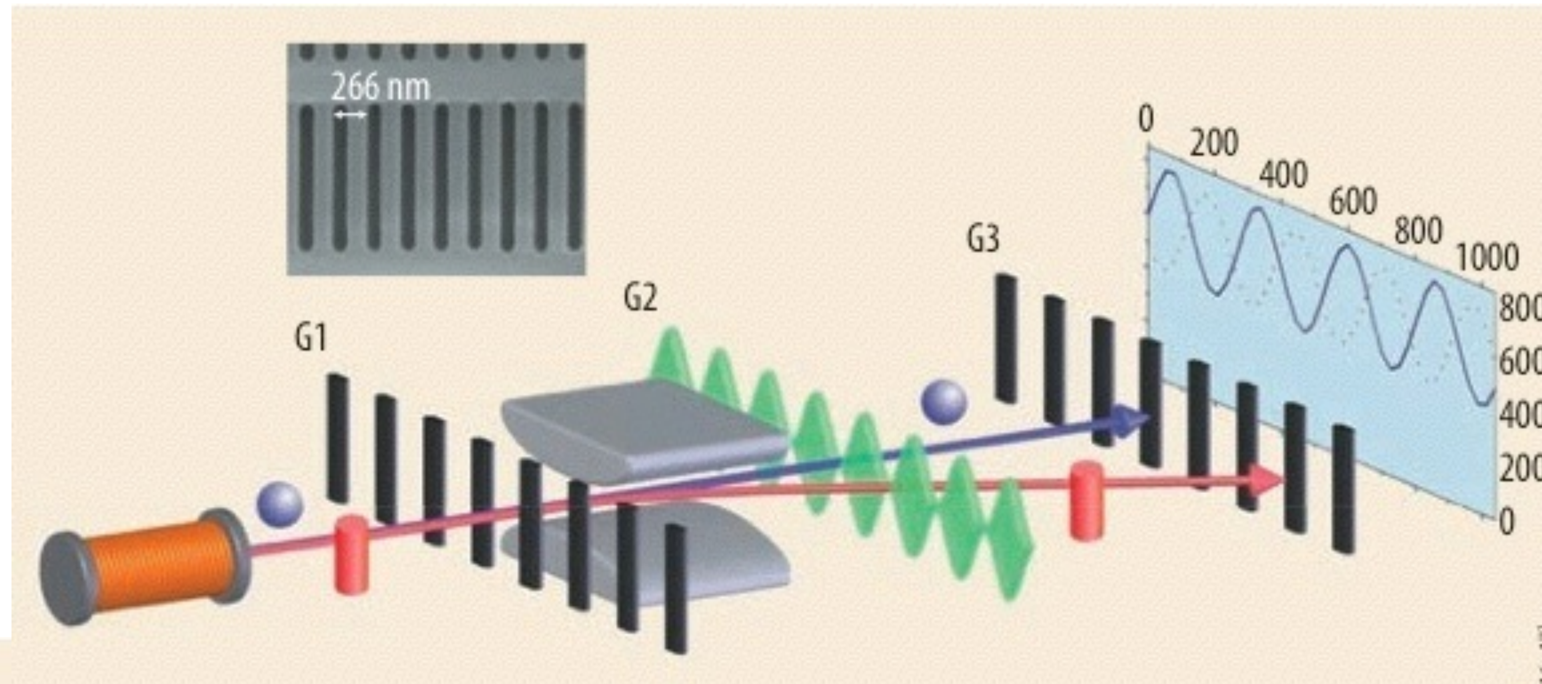
Interferometrie mit komplexen Molekülen

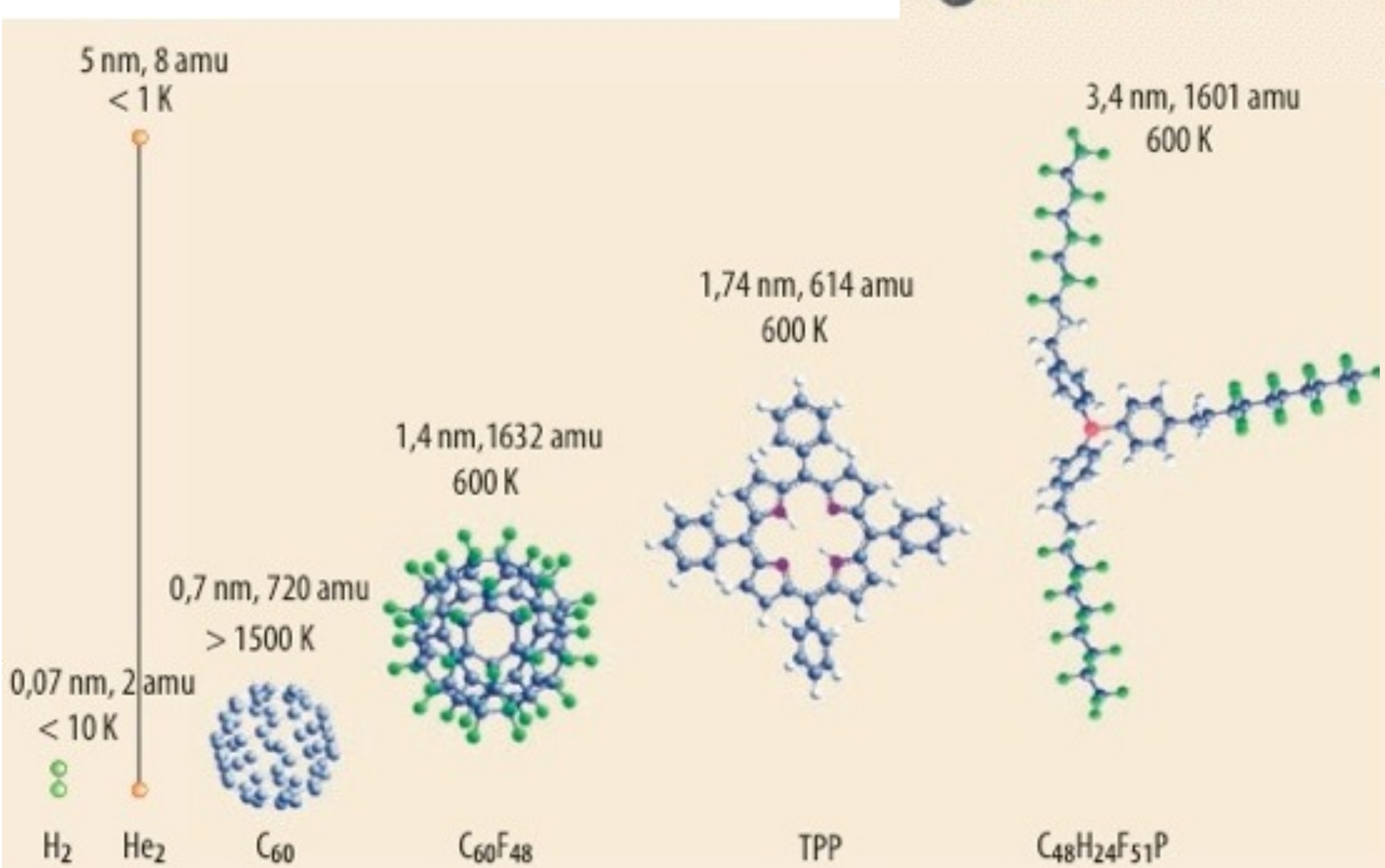
Physik Journal **9** Okt. 2010, p. 37

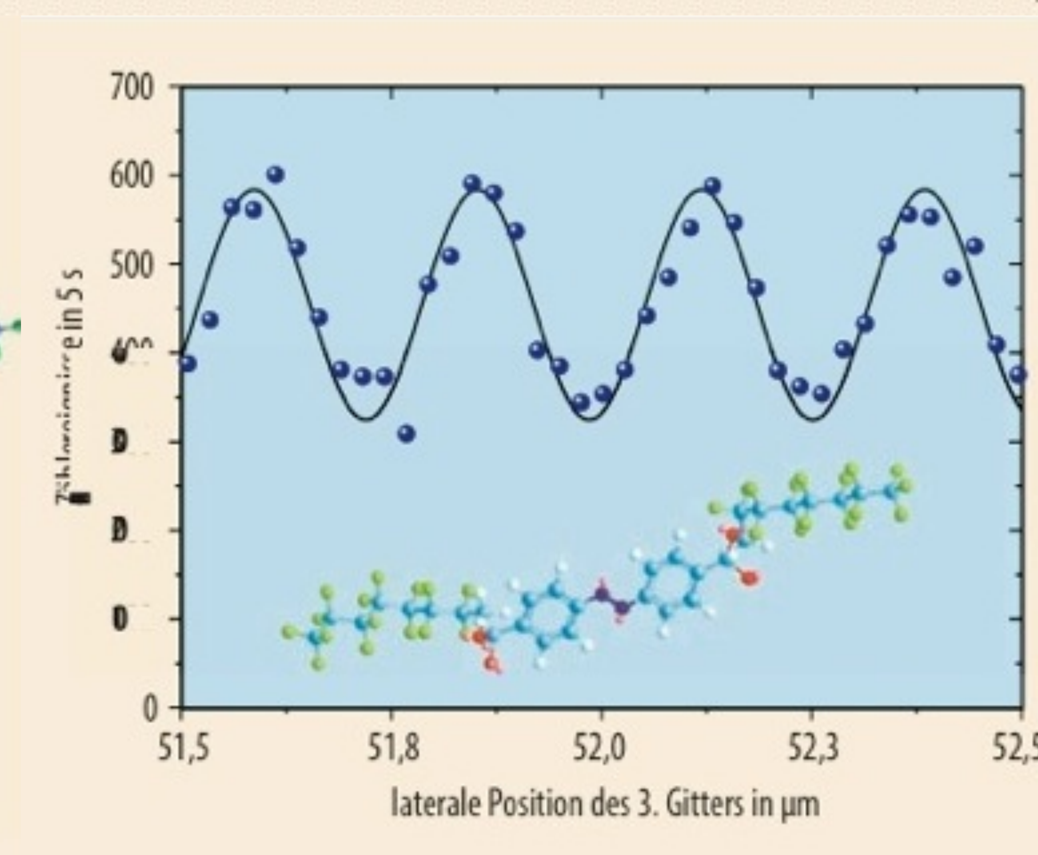
Wie man Einblick in das Innenleben von quantenmechanisch delokalisierten Molekülen gewinnt

Markus Arndt, Stefan Gerlich, Klaus Hornberger und Marcel Mayor

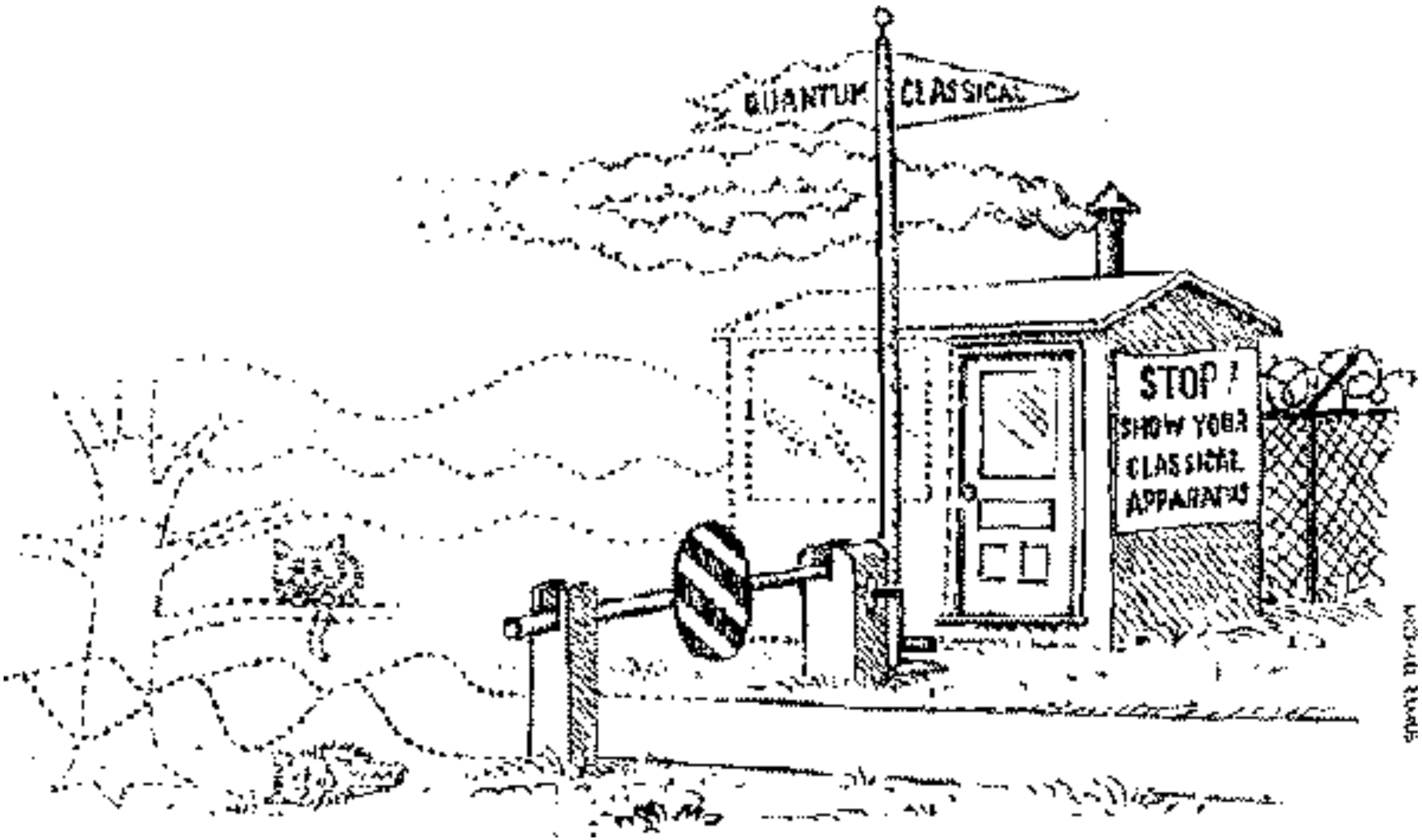
not just electrons behave as waves ...







quantum vs. classical behavior



time-dependent Schödinger equation

particle		wave	dispersion relation		solution $e^{i(kz-\omega t)}$
p	$=$	$\hbar k$	photons	$\omega = ck$	$\frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = \frac{\partial^2\Phi}{\partial z^2}$
E	$=$	$\hbar\omega$	electrons	$E = \frac{p^2}{2m}$	$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2}$

time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r},t)\right)\Psi(\vec{r},t)$$

1st derivative:
complex waves,
initial-value problem:

$$\Psi(\vec{r},t+\delta t) \approx \Psi(\vec{r},t) + \frac{\partial\Psi(\vec{r},t)}{\partial t}\,\delta t$$

separation of variables

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right) \Psi(\vec{r}, t)$$

time-independent potential

ansatz: $\Psi(\vec{r}, t) = A(t) \psi(\vec{r})$

$$i\hbar \frac{\partial A(t)}{\partial t} \psi(\vec{r}) = A(t)\, E\, \psi(\vec{r}) = A(t) \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right) \psi(\vec{r})$$

$$A(t) = A_0\, e^{-iEt/\hbar} \qquad \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right) \psi(\vec{r}) = E\, \psi(\vec{r})$$

time-independent Schrödinger equation
(eigenvalue problem)

general solution: linear combination of eigenstates

$$\Psi(\vec{r}, t) = \sum_n a_n\, e^{-iE_n t/\hbar}\, \psi_n(\vec{r})$$

exercise

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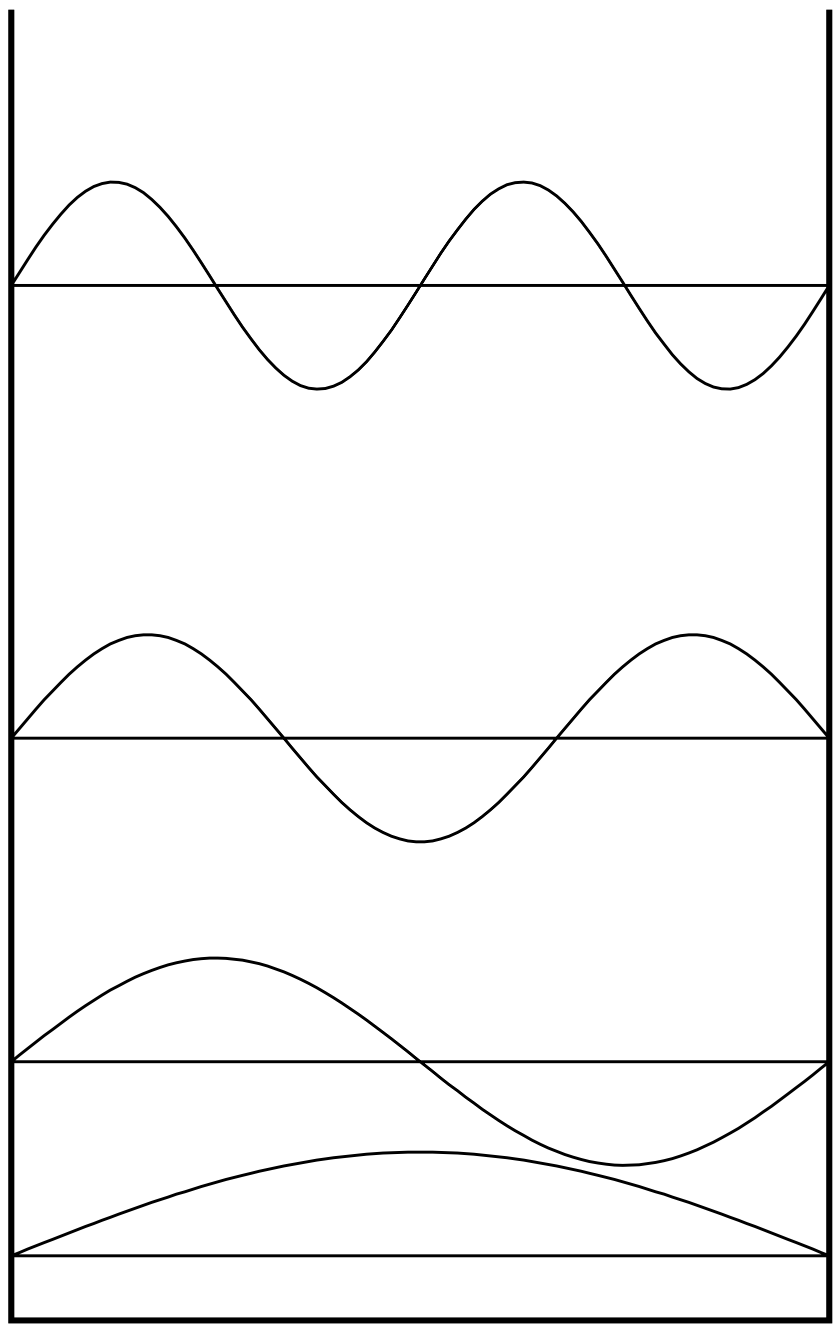
particle in a box



boundary conditions ⇒ **quantization**

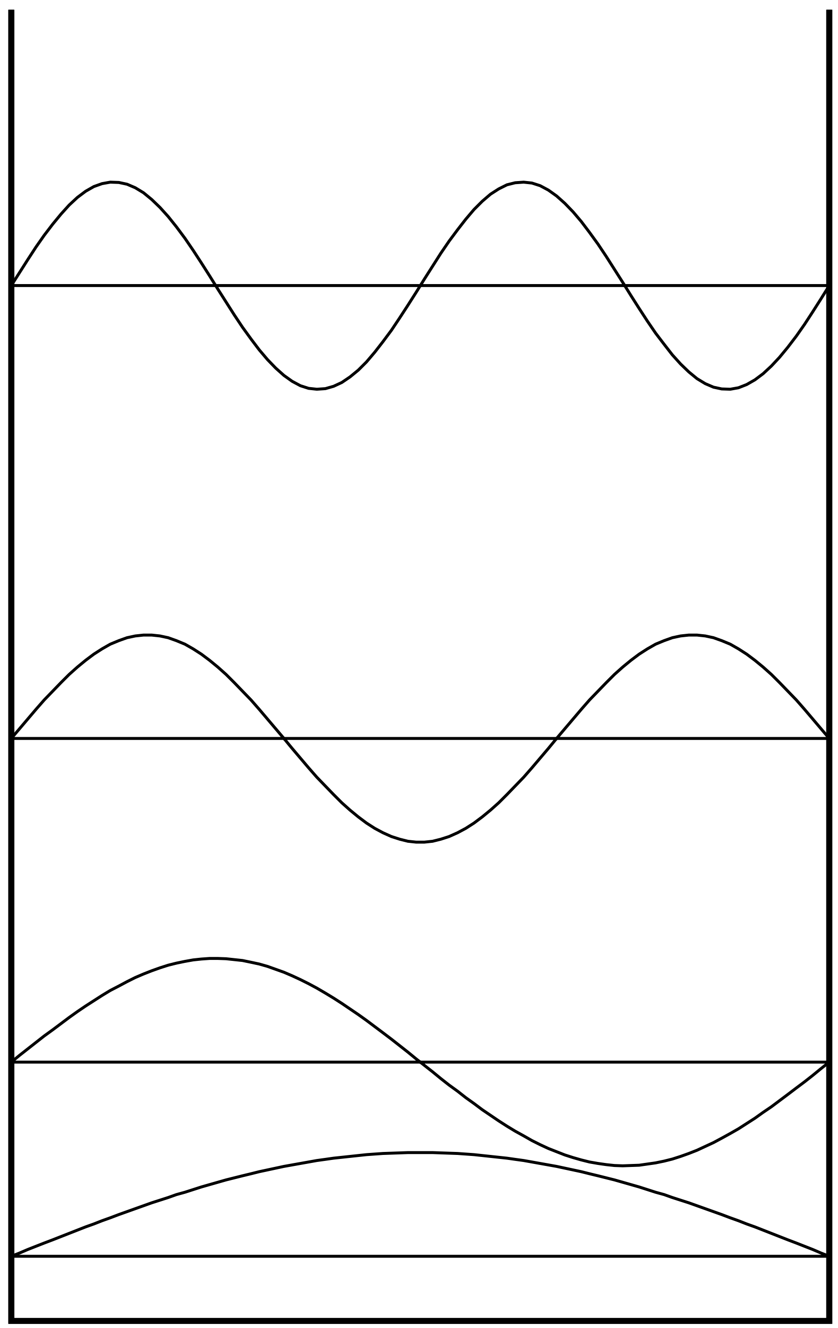
$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2$$

$$\varphi_n(z) = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n\pi\, z}{L_z}\right)$$

discrete energies
zero-point energy
increasing number of nodes

symmetry of potential
symmetry of solutions (density)
even/odd eigenfunctions

particle in a box



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typical units

$h = 6.626068\ 10^{-34}$ Js
$m_{el} = 9.109382\ 10^{-31}$ kg
$e = 1.602176\ 10^{-19}$ C

http://physics.nist.gov/cuu/Constants/index.html

$$E = \frac{\hbar^2\, k^2}{2m_{el}}$$

why use Å and eV?

1 Å $= 10^{-10}$ m
1 eV $= 1.602176\ 10^{-19}$ J

E [in J] $= 6.10\ 10^{-39}$ (k [in m^{-1}])^2

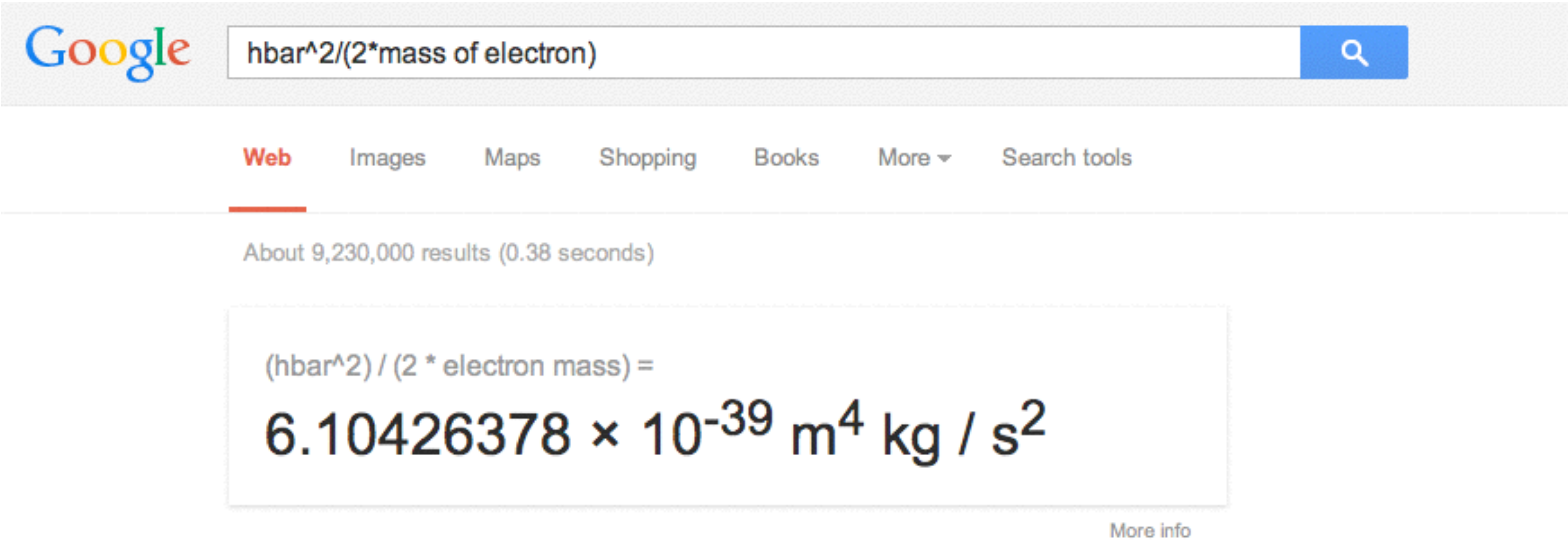
E [in eV] $=$ 3.81 (k [in Å^{-1}])^2

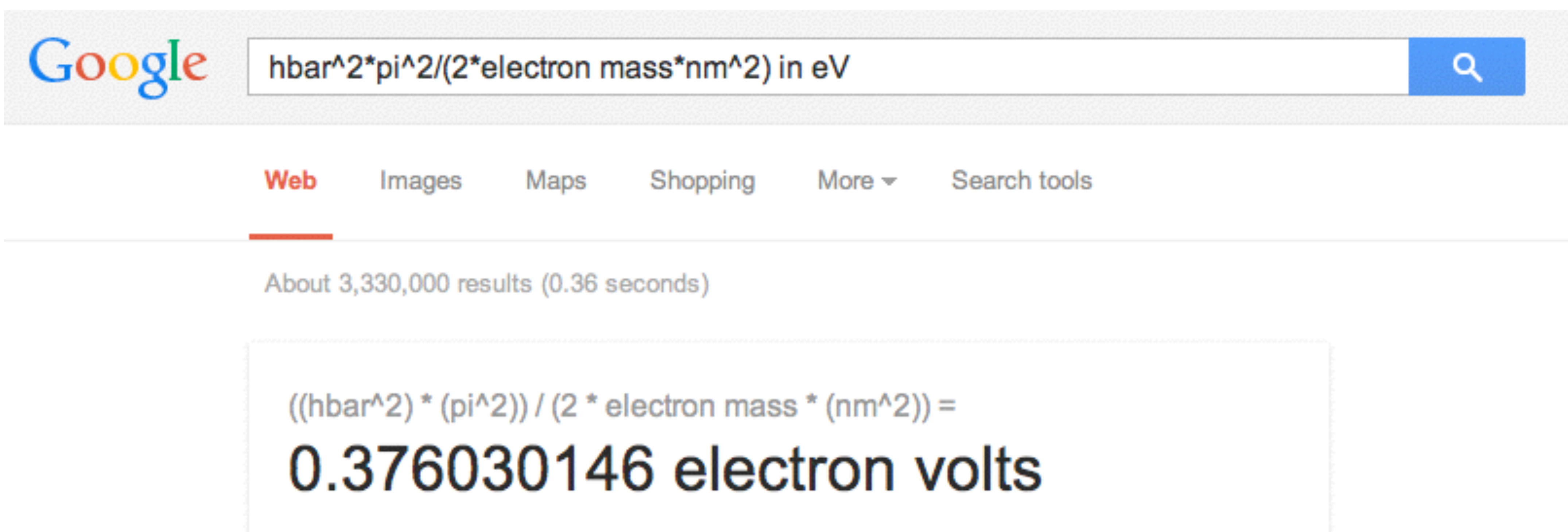
```
from math import pi
hbar  = 1.0546e-34      # h/2pi in Js
me    = 9.1094e-31      # electron mass in kg
e     = 1.6022e-19      # electron charge in C

const=hbar**2/(2*me)    # print(const) --> 6.10457966496e-39
L = 1e-9                # in m (1 nm = 10 \AA)
k1=pi/L
E1=const*k1**2          # ground-state energy --> 6.024979e-20 J

const=hbar**2/(2*me)/(1e-10**2*e) # print(const) --> 3.81012337097
L = 10                  # in \AA
k1=pi/L
E1=const*k1**2          # ground-state energy --> 3.760441e-01 eV
```

calculating with Google





atomic units

$$
\begin{aligned}
\hbar &= 1.0546 \cdot 10^{-34} && \text{Js} && [ML^2T^{-1}] \\
m_e &= 9.1094 \cdot 10^{-31} && \text{kg} && [M] \\
e &= 1.6022 \cdot 10^{-19} && \text{C} && [Q] \\
4\pi\epsilon_0 &= 1.1127 \cdot 10^{-10} && \text{F/m} && [M^{-1}L^{-3}T^2Q^2]
\end{aligned}
$$

`http://physics.nist.gov/cuu/`

solve

$$
\begin{aligned}
\hbar &= 1\; a_0^2\, m_e \,/\, t_0 \\
m_e &= 1\; m_e \\
e &= 1\; e \\
4\pi\epsilon_0 &= 1\; t_0^2\, e^2 \,/\, a_0^3\, m_e
\end{aligned}
$$

to obtain

$$
\begin{aligned}
1 \text{ a.u. length} &= a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \approx 5.2918 \cdot 10^{-11} \text{ m} \\
1 \text{ a.u. mass} &= m_e = \approx 9.1095 \cdot 10^{-31} \text{ kg} \\
1 \text{ a.u. time} &= t_0 = \frac{(4\pi\epsilon_0)^2\hbar^3}{m_e e^4} \approx 2.4189 \cdot 10^{-17} \text{ s} \\
1 \text{ a.u. charge} &= e = \approx 1.6022 \cdot 10^{-19} \text{ C}
\end{aligned}
$$